

# Fall 2009 Cray XT5 Hex-core Workshop



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**Group Leader**

**User Assistance and Outreach**  
**National Center for Computational Sciences**

Oak Ridge, Tennessee  
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U.S. DEPARTMENT OF  
**ENERGY**



**OAK RIDGE NATIONAL LABORATORY**

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

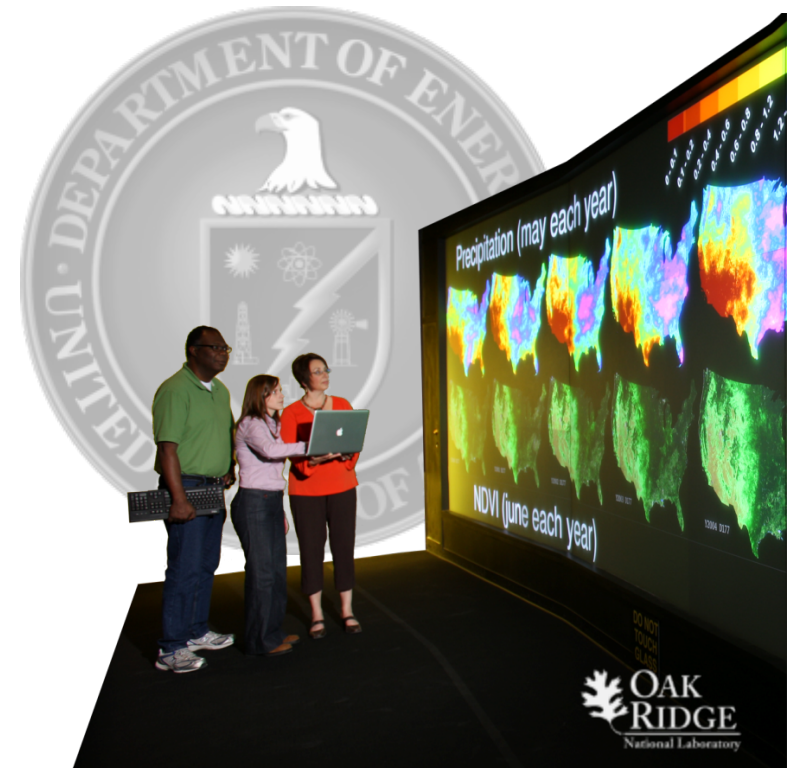
# Welcome to the Fall Hex Core Workshop for **Jaguar** and **Kraken**!



# Oak Ridge Leadership Computing Facility Mission

Our mission is to enable breakthrough science by:

- fielding the most powerful capability computers for scientific research
- building the required infrastructure to facilitate user access to these computers
- working with the DOE to select a few time-sensitive problems of national importance that can take advantage of these systems
- and joining forces with these teams to deliver breakthrough science



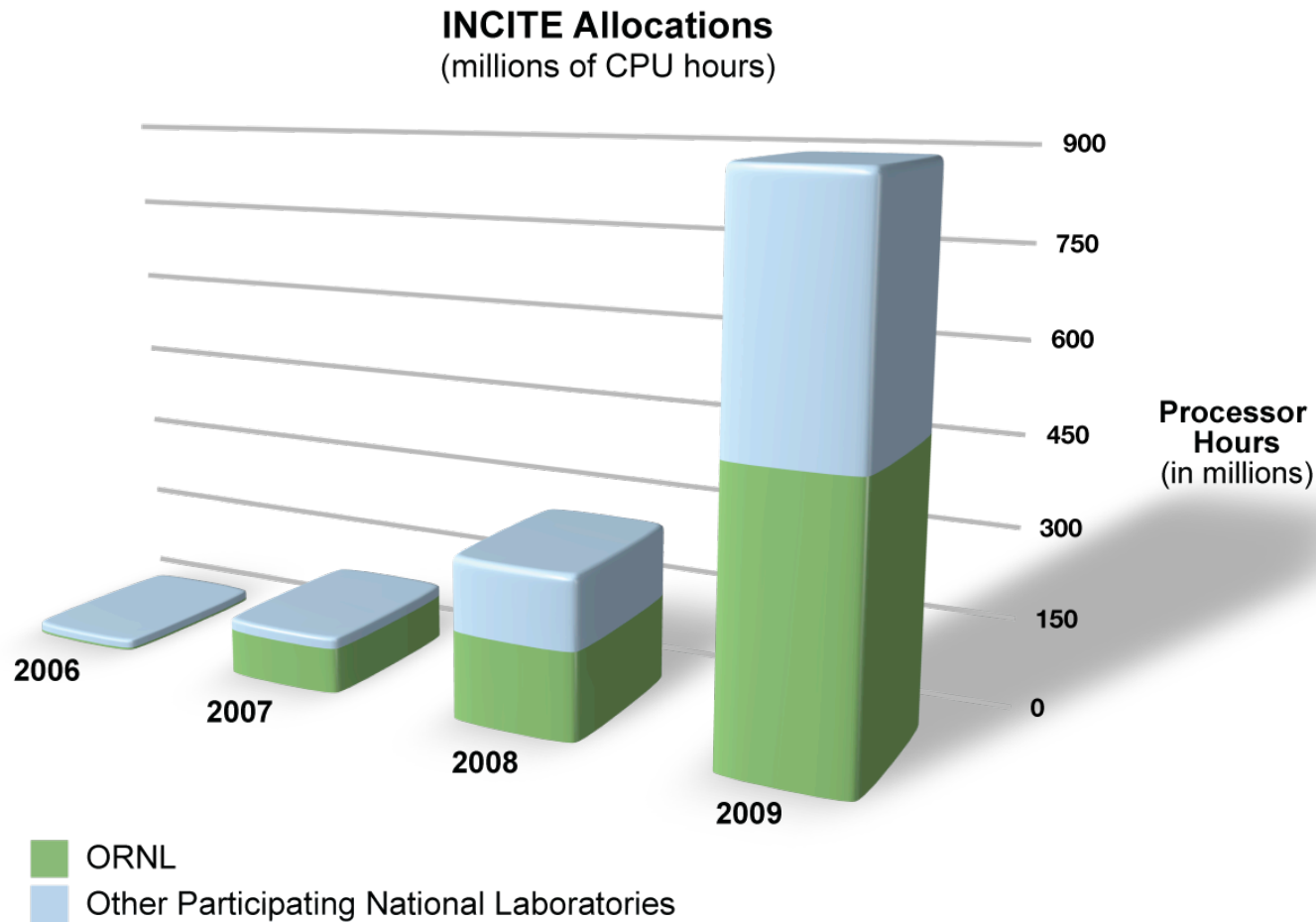
# Jaguar



Peak performance	1.645 petaflops
System memory	362 terabytes
Disk space	10.7 petabytes
Disk bandwidth	240 gigabytes/second

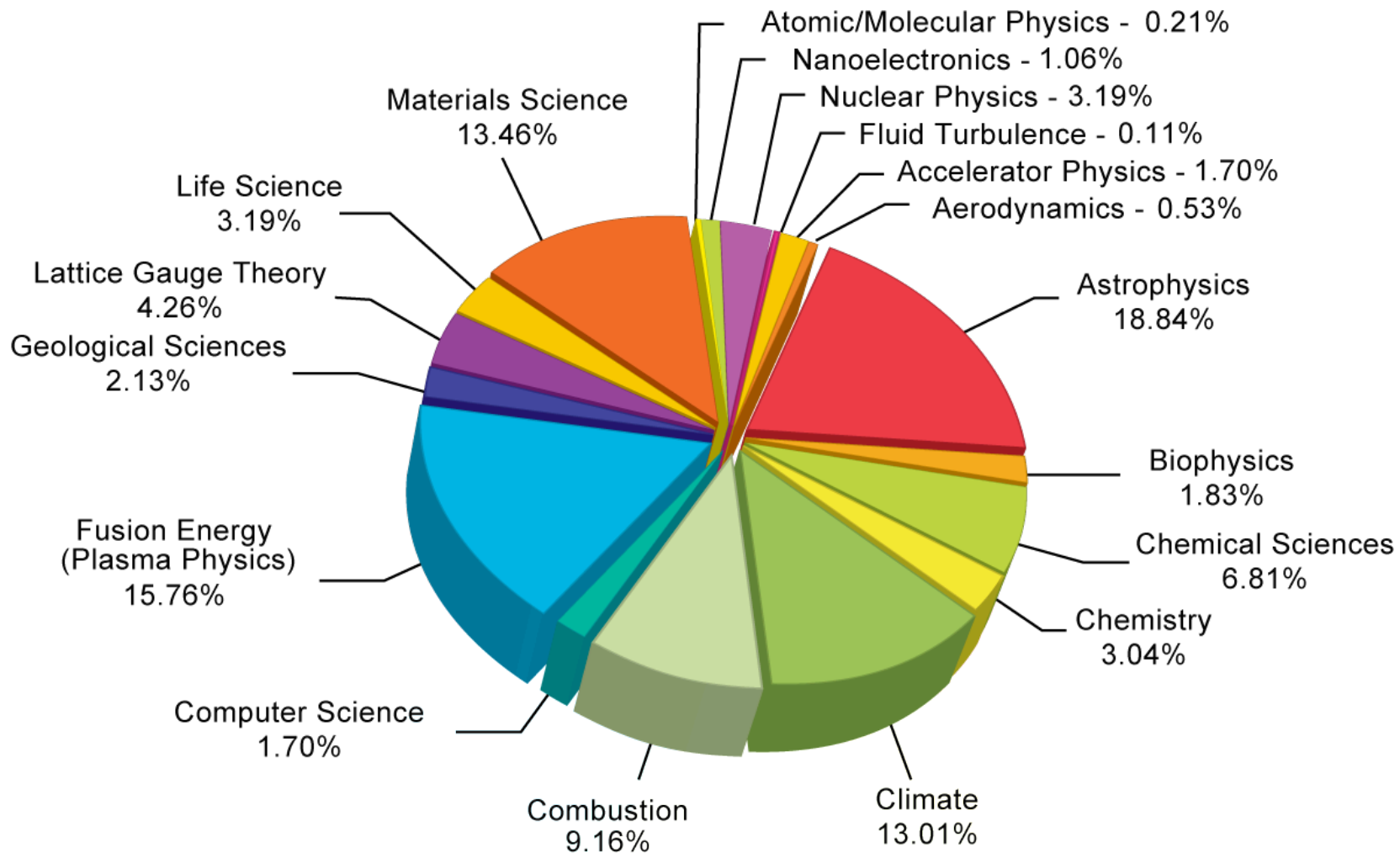
**The XT5 contains 224,256 compute cores in addition to dedicated login/service nodes. Each compute node contains two hex-core AMD Opteron processors, 16GB memory, and a SeaStar 2+ router.**

# Primary Resource Allocation Mechanism: INCITE<sup>†</sup>



<sup>†</sup> Innovative and Novel Computational Impact on Theory and Experiment

# INCITE<sup>†</sup> 2009 Allocations by Discipline



<sup>†</sup> Innovative and Novel Computational Impact on Theory and Experiment



# National Institute for Computational Sciences



- NICS is a collaboration between the University of Tennessee and ORNL
- Awarded the NSF Track 2B (\$65M)
- Phased deployment of Cray XT systems (culminated in 1 PF in October 2009)



# Cray XT5 (Kraken) Upgrade

Compute Processor	AMD 2.3 GHz Barcelona	AMD 2.6 GHz Istanbul
Compute cores	66,048	99,072
Compute sockets	16,512 quad-core	16,512 hex-core
Compute nodes	8,256	8,256
Memory per node	8 GB on 3,840 nodes 16 GB on 4,416 nodes	16 GB (all nodes)
Total memory	100 TB	129 TB
Parallel file system space	3.3 PB (raw)	3.3 PB (raw)
Peak system performance	0.608 PF	1.03 PF





# Cray XT5 (Kraken) Upgrade

## SELECTED NSF ALLOCATIONS AT NICS

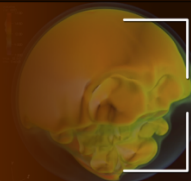
NATIONAL SCIENCE FOUNDATION AND NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES  
TERAGRID RESOURCE ALLOCATION COMMITTEE (TRAC) AWARDS - 2009



NICS

### 3D Stellar Core Collapse

PI: Bronson Messer  
University of Tennessee/Oak Ridge National Laboratory - 9,700,000 hours



### Scaling in Turbulence and Turbulence Mixing

PI: Pui-Kuen Yeung  
Georgia Institute of Technology - 5,843,000 hours



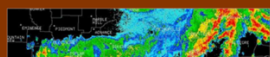
### SCEC Rupture Dynamics Code Validation

PI: Thomas Jordan  
University of Southern California - 11,500,000 hours



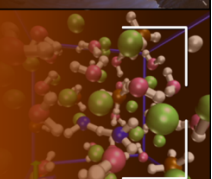
### Predicting Continental US Scale Weather at 1 km in Real Time with Full-Scale Radar Data Assimilation

PI: Ming Xue  
University of Oklahoma - 3,382,000 hours



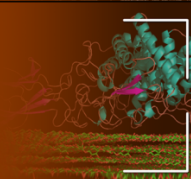
### Ab-initio Molecular Dynamics Investigation of Complex Hydride Kinetics

PI: Christopher Wolverton  
Northwestern University - 1,000,000 hours



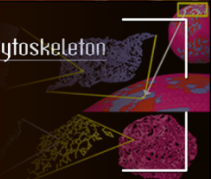
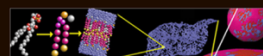
### Understanding Cellulosic Ethanol through High-Performance Computing

PI: Jeremy Smith  
University of Tennessee/Oak Ridge National Laboratory Center for Molecular Biophysics - 2,400,000 hours



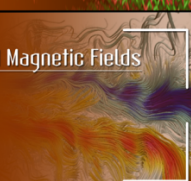
### Large-Scale Molecular Dynamics Simulation of a Key Element of the Cellular Cytoskeleton

PI: Gregory Voth  
University of Utah - 8,995,000 hours



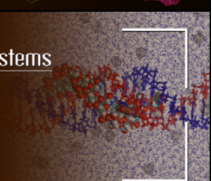
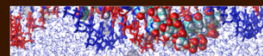
### Coupling of Turbulent Compressible Solar Convection with Rotation, Shear and Magnetic Fields

PI: Juri Toomre  
University of Colorado - 15,000,000 hours



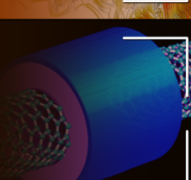
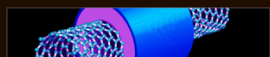
### Atomic Level Contributions to Structural and Dynamic Properties of Biological Systems

PI: Alexander MacKerell, Jr.  
University of Maryland, School of Pharmacy - 540,000 hours



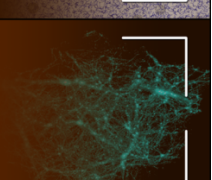
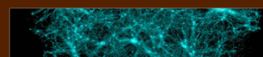
### Atomistic Simulations of Future Nanoelectronics Transistors

PI: Matheiu Luisier  
Purdue University - 10,300,000 hours



### ENZO: Simulating the Early Universe

PI: Alexei Kritsuk  
University of California-San Diego - 4,100,000 hours



# Day 1 - Morning

Time	Topic	Speakers
8:00 AM	Morning coffee	
8:15 – 8:30 AM	Welcome and Intro to the Workshop	Ashley Barker NCCS UAO Group Lead
8:30 – 9:00 AM	Cray Roadmap Update	Jeff Larkin, Cray
9:00-10:00 AM	Description of AMD 6-core CPU for Application Developers	Brian Waldecker, AMD Staff
10:00 – 10:15 AM	Break	
10:15 – 10:45 AM	Cray XT Architecture-detailed description of Cray XT5 systems, including interconnect and node	Jeff Larkin, Cray
10:45 – 11:45 AM	Overviews of Kraken and Jaguar	Daniel Lucio, NICS Staff Donald Frederick, NCCS Staff
Noon – 1:00 PM	Working Lunch	Kittrich Sheets, Cray

# Day 1 – Afternoon

Time	Topic	Speakers
1:00 – 2:00 PM	Using CrayPAT to measure application performance	Luiz DeRose, Cray, Inc
2:00 – 5:00 PM	Hands-on Session Intro to using NCCS/NICS/XT5 6-core systems	NCCS/NICS/Cray Staff

## Day 2 - Morning

Time	Topic	Speakers
8:00 AM	Working breakfast to allow participants to discuss their work for the day's meeting, Continue working on previous day's materials	
8:15 – 9:15 AM	Specific Optimizations for the Cray XT5 6-Core Systems	Jeff Larkin, Cray, Inc.
9:15 – 10:00 AM	How to Make the Best Use of Cray MPI	Kim McMahon, Cray, Inc.
10:00-10:15 AM	Break	
10:15 – 11:00 AM	Using Cray MPI – An Application Developer's Perspective	Mark Fahey, NICS
11:00 – 11:45 AM	The Cray Scientific Libraries	Cray Staff, Cray, Inc.
Noon – 1:00 PM	Working lunch – review of morning materials, Question and Answers; Presentation on application experience on XT systems : User Experience Topic: TBA	TBA

## Day 2 - Afternoon

Time	Topic	Speakers
1:00 – 2:00 PM	Introduction to Cray Compilers	Nathan Wichman, Cray
2:00 – 3:00 PM	Using PGI Compilers	PGI Staff
3:00 -3:15 PM	Break	
3:15 – 3:45 PM	Introduction to Lustre and NCCS Spider Parallel file systems for XT5	David Dillow, NCCS
3:45 -4:15 PM	Using I/O on Cray XT Systems	Lonnie Crosby, NCCS
4:15 – 5:00 PM	Using a High-Level I/O library for Improved Performance: ADIOS	Jay Lofstead, Georgia Tech



# Day 3

Time	Topic	Speakers
8:00 AM	Working breakfast to allow participants to discuss their work for the day's meeting, Continue working on previous day's materials	
8:15– 9:15 AM	Introduction to OpenMP on the XT5	Christian Halloy, NICS
9:15– 10:15AM	Using Debuggers on XT5: TotalView	Totalviewtech Staff
10:15 -10:30 AM	Break	
10:30 -11:30 AM	Using Debuggers on XT5: DDT	Allinea Staff
11:45 - 1:00 PM	Working lunch – review of morning materials, Question and Answers; Presentation on application experience on XT systems : User Experience Topic: TBA	TBA
1:00 – 2:00 PM	Parallel Analysis and Visualization on the Cray Linux Environment	Sean Ahern, NCCS
2:00 – 5:00 PM	Hands-on Session Intro to using NCCS/NICS/XT5 6- core systems	NCCS/NICS/Cray Staff